County of San Diego
Air Pollution Control District

Procedures for Estimating the Vapor Pressure of VOC Mixtures
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Estimating the vapor pressure of solvents that are blends of several VOCs will require either the volume or weight percentage of every component of the mixture be available from the manufacturer's specifications or from material safety data sheets. The calculation method in this procedure provides a value to be used in rule compliance determination for the vapor pressure of a mixture when there is no vapor pressure data for the mixture available. Results that are near rule limits and were obtained using this procedure may need additional evaluation.

The estimate uses the approximations that the liquid solution behaves as an ideal solution and that the gas phase behaves as an ideal gas. The calculation involves converting volume or weight percentage data to mole fractions of the liquid mixture and using these mole fractions and pure component vapor pressures to estimate the vapor pressure of the mixture at a temperature. The calculation may not apply to water-based mixtures or emulsions/suspensions. In this calculation, the portion of the vapor pressure of the mixture contributed by exempt solvents, i.e. 1,1,1-trichloroethane and others as stipulated in the definition of VOC, will not be included in arriving at a mixture vapor pressure. Pure component vapor pressure is available from a variety of references. Additionally, vapor pressure data for specific mixtures may be available from the manufacturer of the mixture and also may be found in material data files in the engineering division. If the manufacturer's vapor pressure data are used, the source of the data and test method need to be verified to substantiate using this data.

A. When using volume percentage of the liquid mixture, follow this procedure:

1) Check that the volume percentages add up to 100.

2) Convert the volume percentage to a fraction by dividing each by 100.

[Volume fraction] comp. = [Volume percent] comp./100

3) Convert the volume fraction to weight per gallon of mixture by multiplying the volume fraction by the density of the component of the mixture.

[Weight per gallon] comp. = [Volume fraction] comp. x [Density] comp.

4) Convert the weight of component per gallon of mixture to moles of component per gallon of mixture by dividing by the molecular weight of the component.

[Moles per gallon] comp. =
[Weight per gallon] comp. / [Molecular weight] comp.

5) Sum the number of moles of the individual components of the mixture.

Σ [Moles] = [Moles] comp. A + [Moles] comp. B + ... + [Moles] last comp.

6) Calculate the mole fraction of each component by dividing the number of moles of a component by the total number of moles obtained from the previous step.

[Mole fraction] comp. = [Moles] comp. / Σ [Moles]

7) Repeat the calculation in the previous step for each component.

8) Add the mole fractions of all the components of the mixture. This should be equal to 1. If it is not equal to 1, the total may be recalculated equal to 1 by multiplying the component mole fraction by the ratio of 1 to the total of all the component mole fractions.

[Mole fraction] comp. (normalized to 1) =
[Mole fraction] comp. x 1/ Σ [Mole fraction] comp.

9) To calculate the vapor pressure of the component of the mixture, multiply the vapor pressure of the pure component at the desired temperature specified by the rule times the mole fraction of the component in the liquid mixture.

[Vapor pressure] comp. in mix. =
[Vapor pressure] comp. pure x [Mole fraction] comp.

10) The total vapor pressure of the mixture is the sum of the vapor pressures of the components in the mixture.

[Vapor pressure] total mix. = Σ [Vapor pressure] comp. in mix.
and [Vapor pressure] VOC = Σ [Vapor pressure] VOC comp.

B. When using weight percentage, follow this procedure:

1) Check that the weight percentages add up to 100.

2) Convert the weight percentage to a fraction by dividing each by 100.

[Weight fraction] comp. = [Weight percent] comp. /100

3) Convert the weight fraction of the component to weight per gallon of the component by multiplying by the density of the mixture.

[Weight per gallon] comp. = [Weight fraction] comp. x [Density] mix.

Then follow Steps *4)* through *10).*